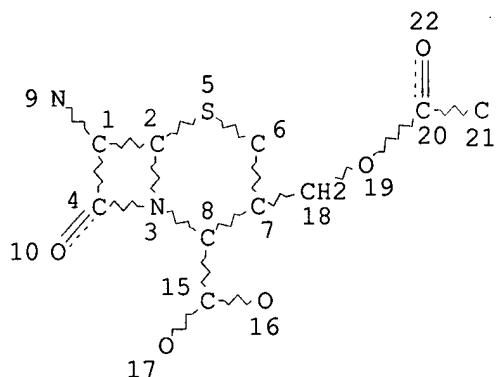


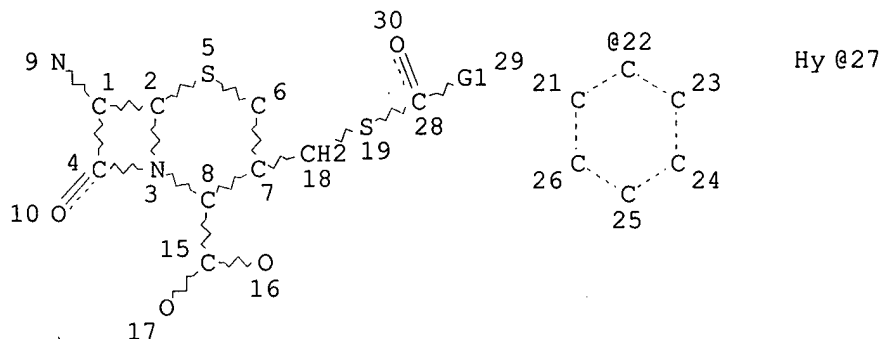
=> d que stat 125
L13 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
L17 STR



VAR G1=22/27
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

(C) STEREO ATTRIBUTES: NONE
L18 1 SEA FILE=REGISTRY ABB=ON "BORON TRIFLUORIDE"/CN
L19 1 SEA FILE=REGISTRY ABB=ON 7637-07-2/RN
L21 9929 SEA FILE=REGISTRY SSS FUL L13
L23 345 SEA FILE=REGISTRY SSS FUL L17
L24 1 SEA FILE=REGISTRY ABB=ON L18 OR L19
L25 1 SEA FILE=HCAPLUS ABB=ON L21 AND L23 AND (L24 OR BORON TRIFLUORIDE OR BF3)

=> d 127 ibib abs hitstr 1

L27 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:409294 HCAPLUS

DOCUMENT NUMBER: 136:401577

TITLE: Process for the preparation of Furaca, a useful intermediate for synthesis of cephalosporin antibiotics

INVENTOR(S): Kumar, Uthira; Sivakumaran, Meenakshisunderam; Handa, Vijay Kumar

PATENT ASSIGNEE(S): India

SOURCE: U.S. Pat. Appl. Publ., 3 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

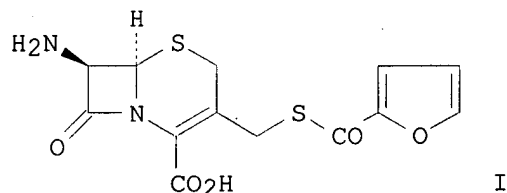
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002065412	A1	20020530	US 2001-902512	20010709

OTHER SOURCE(S): CASREACT 136:401577
GI



AB A process is disclosed for the prepn. of 7-amino-3-(2-furanylcarbonylthiomethyl)-3-cephem-4-carboxylic acid (I), a.k.a. Furaca, via nucleophilic displacement of the acetoxy group of 7-aminocephalosporanic acid by 2-thiofuroic acid. I is useful as an intermediate for the prepn. of ceftiofur cephalosporin antibiotic used for treating bovine respiratory infections. Thus, using sodium sulfide 2-furoyl chloride was converted to 2-thiofuroic acid which was then reacted with 7-aminocephalosporanic acid using **boron trifluoride** in EtOAc to give I in 86% yield.

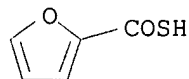
IT 4741-45-1P, 2-Thiofuroic acid

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(process for the prepn. of Furaca, a useful intermediate for synthesis of cephalosporin antibiotics, via a nucleophilic substitution reaction)

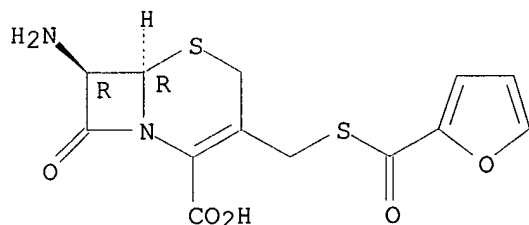
RN 4741-45-1 HCAPLUS

CN 2-Furancarbothioic acid (9CI) (CA INDEX NAME)

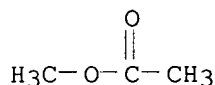


IT **80370-59-8P**, Furaca
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
 (Preparation)
 (process for the prepn. of Furaca, a useful intermediate for synthesis
 of cephalosporin antibiotics, via a nucleophilic substitution reaction)
 RN 80370-59-8 HCAPLUS
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-amino-3-[[(2-furanylcarbonyl)thio]methyl]-8-oxo-, (6R,7R)- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.



IT **79-20-9**, Methyl acetate **108-21-4**, Isopropyl acetate
123-86-4, Butyl acetate **141-78-6**, Ethyl acetate, uses
 RL: NUU (Other use, unclassified); USES (Uses)
 (process for the prepn. of Furaca, a useful intermediate for synthesis
 of cephalosporin antibiotics, via a nucleophilic substitution reaction)
 RN 79-20-9 HCAPLUS
 CN Acetic acid, methyl ester (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 108-21-4 HCAPLUS
 CN Acetic acid, 1-methylethyl ester (9CI) (CA INDEX NAME)

i-Pr-O-Ac

RN 123-86-4 HCAPLUS
 CN Acetic acid, butyl ester (8CI, 9CI) (CA INDEX NAME)

n-Bu-O-Ac

RN 141-78-6 HCAPLUS
 CN Acetic acid ethyl ester (8CI, 9CI) (CA INDEX NAME)

Et-O-Ac

IT **11111-12-9DP**, Cephalosporin, derivs. **80370-57-6P**,
 Ceftiofur
 RL: PNU (Preparation, unclassified); PREP (Preparation)

(process for the prepn. of Furaca, a useful intermediate for synthesis of cephalosporin antibiotics, via a nucleophilic substitution reaction)

RN 11111-12-9 HCAPLUS

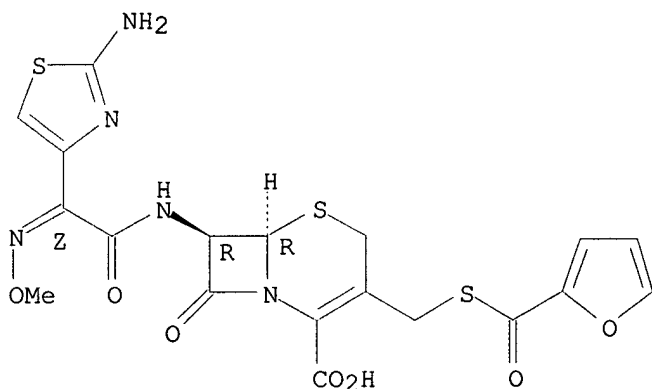
CN Cephalosporin (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 80370-57-6 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[[(2Z)-(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-3-[[2-furanylcarbonyl)thio]methyl]-8-oxo-, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



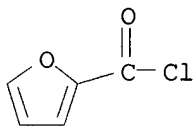
IT 527-69-5, 2-Furoyl chloride 957-68-6,
7-Aminocephalosporanic acid

RL: RCT (Reactant); RACT (Reactant or reagent)

(process for the prepn. of Furaca, a useful intermediate for synthesis of cephalosporin antibiotics, via a nucleophilic substitution reaction)

RN 527-69-5 HCAPLUS

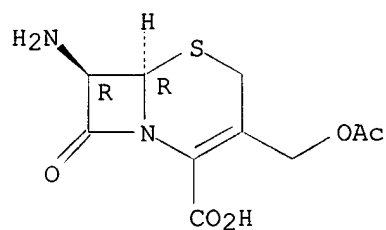
CN 2-Furancarbonyl chloride (9CI) (CA INDEX NAME)



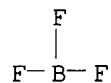
RN 957-68-6 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[(acetyloxy)methyl]-7-amino-8-oxo-, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 7637-07-2, **Boron trifluoride**, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(process for the prepn. of Furaca, a useful intermediate for synthesis
of cephalosporin antibiotics, via a nucleophilic substitution reaction)
RN 7637-07-2 HCAPLUS
CN Borane, trifluoro- (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 14:32:48 ON 29 JUL 2002)

FILE 'REGISTRY' ENTERED AT 14:44:12 ON 29 JUL 2002
ACT BER074STR/L

L1 STR
L2 STR L1
L3 7 S L2
L4 122 S L3 FULL

FILE 'HCAPLUS' ENTERED AT 14:48:43 ON 29 JUL 2002
L5 798 S L4

FILE 'REGISTRY' ENTERED AT 14:55:16 ON 29 JUL 2002
L6 STR L2
L7 SCREEN 2039
L8 2 S L6 NOT L7
L9 33 S L6 NOT L7 FULL

FILE 'HCAPLUS' ENTERED AT 15:09:35 ON 29 JUL 2002
L10 792 S L9

FILE 'REGISTRY' ENTERED AT 15:13:23 ON 29 JUL 2002
SAVE L9 BER074REG/A

FILE 'HCAPLUS' ENTERED AT 15:13:31 ON 29 JUL 2002
SAVE L10 BER074HCA/A
L11 88 S L10 AND (PREP? OR SYNTH? OR PURIF? OR CRYSTALLIZ?)

FILE 'HCAPLUS' ENTERED AT 15:41:30 ON 29 JUL 2002

FILE 'MEDLINE, BIOSIS, EMBASE, WPIDS, JICST-EPLUS, JAPIO' ENTERED AT
15:41:54 ON 29 JUL 2002
L12 4 S 84085780/AN

FILE 'REGISTRY' ENTERED AT 16:57:33 ON 29 JUL 2002
ACT BER178A/A

L13 STR
L14 9929 SEA FILE=REGISTRY SSS FUL L13

ACT BER178B/A

L15 STR
L16 19275 SEA FILE=REGISTRY SSS FUL L15

L17 STR L15

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L18 1 S "BORON TRIFLUORIDE"/CN
L19 1 S 7637-07-2/RN
L20 50 S L13
L21 9929 S L13 FULL
L22 16 S L17
L23 345 S L17 FULL
L24 1 S L18 OR L19

FILE 'HCAPLUS' ENTERED AT 17:09:10 ON 29 JUL 2002
L25 1 S L21 AND L23 AND (L24 OR BORON TRIFLUORIDE OR BF3)

FILE 'REGISTRY' ENTERED AT 17:13:00 ON 29 JUL 2002

FILE 'HCAPLUS' ENTERED AT 17:13:32 ON 29 JUL 2002
SELECT RN L25 1

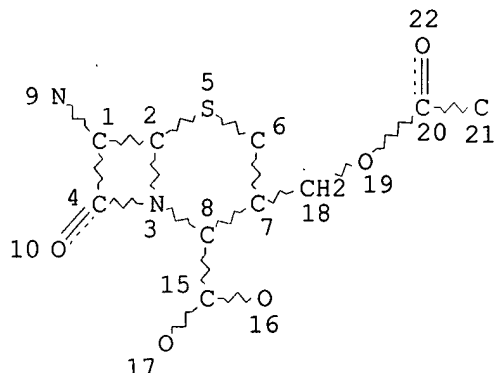
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L26 11 S E1-11

FILE 'HCAPLUS' ENTERED AT 17:13:56 ON 29 JUL 2002
L27 1 S L25 AND L26
SAVE L27 BER178HCA/A
SAVE L17 BER178STRB/L
L28 4966 S L19

FILE 'REGISTRY' ENTERED AT 17:21:30 ON 29 JUL 2002
L29 1 S L18 OR L19 OR L28
L30 1 S L27 OR L29

FILE 'HCAPLUS' ENTERED AT 17:23:09 ON 29 JUL 2002

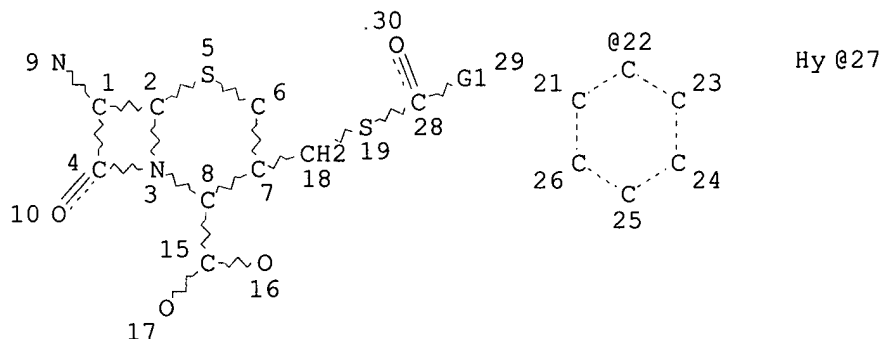
=> d que stat 127
L13 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
L17 STR



VAR G1=22/27
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L18 1 SEA FILE=REGISTRY ABB=ON "BORON TRIFLUORIDE"/CN
L19 1 SEA FILE=REGISTRY ABB=ON 7637-07-2/RN
L21 9929 SEA FILE=REGISTRY SSS FUL L13
L23 345 SEA FILE=REGISTRY SSS FUL L17
L24 1 SEA FILE=REGISTRY ABB=ON L18 OR L19
L25 1 SEA FILE=HCAPLUS ABB=ON L21 AND L23 AND (L24 OR BORON TRIFLUORIDE OR BF3)
L26 11 SEA FILE=REGISTRY ABB=ON (108-21-4/BI OR 11111-12-9/BI OR

123-86-4/BI OR 141-78-6/BI OR 4741-45-1/BI OR 527-69-5/BI OR
7637-07-2/BI OR 79-20-9/BI OR 80370-57-6/BI OR 80370-59-8/BI
OR 957-68-6/BI)

L27

1 SEA FILE=HCAPLUS ABB=ON L25 AND L26